

Amendments to the Claims:

This listing of claims will replace all prior versions, and listings, of claims in the application:

Listing of Claims:

1. (Currently Amended) A parallel computing method for executing calculation of the Hartree-Fock method in a molecular orbital method for a target molecule of a biological material, comprising the steps of:

using a computer cluster made up of a plurality of computers and a communication device coupled to said plurality of computers, each of said plurality of computers comprising a matrix storage having a memory capacity which is insufficient to store whole matrices used in Hartree-Fock calculation;

dividing a density matrix, which is defined by molecular orbital coefficients of the target molecule, into multiple density submatrixes and distributing the multiple density submatrixes to the multiple computers and storing ~~therein~~ the distributed multiple density matrixes in the respective matrix storages; [[and]]

executing, in parallel in the plurality of the computers, calculation processes including two-electron integrations on the density submatrixes stored in the matrix storages [[each]] of the respective computers to update the stored density submatrixes based on the result of the two-election integration; and

[[while]] in each of the computers sequentially transferring the multiple density submatrixes stored in the matrix storage to one of other computers according to order of transfer between the multiple computers via said communication device, and storing the density submatrixes, which are transferred thereto via said communication device, in the matrix storage,

wherein the executing and transferring steps are repeated at the number of times which corresponds to the number of the computers to subject all of the density submatrixes to the calculation processes by sequentially transferring the density submatrixes between the computers, and a Fock matrix of the target molecule is obtained by adding an H-core matrix to the combination of resultant submatrixes stored in said matrix storages of said plurality of computers.

2. (Previously Presented) The method according to Claim 1, wherein a duplication of the density matrix is used, and the density matrix and the duplication are individually divided into density submatrixes, causing the density submatrixes to transfer between the computers via said communication device to thereby reduce calculation of integrals.

3. (Previously Presented) The method according to Claim 1, wherein the density matrix and duplications of the density matrix, four in total, are used, and the density matrix and the duplications are individually divided into density submatrixes, causing the density submatrixes to transfer between the computers via said communication device, to thereby reduce calculation of integrals, by using symmetry of $(rs|tu) \Leftrightarrow (tu|rs)$ in two-electron integration.

4. - 6. (Canceled).

7. (Currently Amended) A parallel computing system for executing calculation of the Hartree-Fock method in a molecular orbital method for a target molecule of a biological material, comprising:

a computer cluster made up of a plurality of computers and a communication device coupled to said plurality of computers,

each of the computers comprising a matrix storage for storing density submatrixes which are divided from a density matrix, which is defined by molecular orbital coefficients of the target molecule; a transfer controller for performing transmission and reception of the density submatrixes with respect to the other computers in the computer cluster; and a calculation processor for performing a calculation process on the density submatrix stored in the matrix storage,

wherein said each matrix storage has a memory capacity which is insufficient to store whole matrices used in Hartree-Fock calculation,

wherein the density matrix is divided into multiple density submatrixes, and the multiple submatrixes are distributed to the multiple computers and stored in initial values of

~~the density submatrices are supplied to the matrix stages storages~~ of the respective computers as initial values,

wherein calculation processes including two-electron integrations on the density submatrices are executed in [[each]] parallel in the plurality of the computers while the multiple density submatrices are being sequentially transferred between the multiple computers via said communication device, wherein, in each of the computers, the density submatrices stored in the matrix storage is transferred to one of other computers according to order of transfer, and the density submatrices which are transferred thereto are store in the matrix storage,

wherein the execution of the calculation processes and transferring are repeated at the number of times which corresponds to the number of the computers to subject all of the density submatrices to the calculation processes, and

wherein a resultant Fock matrix of the target molecule is can be obtained by adding an H-core matrix to the combination of combining resultant [[Fock]] submatrices stored in said matrix storages of said plurality of computers.

8. (Previously Presented) The system according to Claim 7, wherein said storage stores two groups of the density submatrices which are obtained by individually dividing the density matrix and a duplication of the density matrix, the two groups of the density submatrices are transferred between the computers via said communication device, to thereby reduce calculation of integrals.

9. (Previously Presented) The system according to Claim 7, wherein said storage stores four groups of the density submatrices which are obtained by individually dividing the density matrix and duplications of the density matrix, four in total, and the four groups of the density submatrices are transferred between the computers via said communication device, to thereby reduce calculation of integrals, by using symmetry of $(rs|tu) \leftrightarrow (tu|rs)$ in two-electron integration.

10. - 12. (Canceled).

13. (Currently Amended) A computer readable medium storing a computer program causing a computer at each node in a computer cluster constituted by a plurality of nodes and a communication device coupled to said plurality of nodes, to function as:

a matrix storage for storing density submatrixes which are divided from a density matrix; which is defined by molecular orbital coefficients of a target molecule of a biological material; a transfer controller for performing transmission and reception of the density submatrixes with respect to the other nodes in the computer cluster; and a calculation processor for performing a calculation process on the density submatrix stored in the matrix storage,

whereby said each matrix storage has a memory capacity which is insufficient to store whole matrices used in Hartree-Fock calculation,

whereby the density matrix is divided into multiple density submatrixes, and the multiple submatrixes are distributed to the multiple computers and stored in initial values of the density submatrixes are supplied to the matrix stages storages of the respective nodes as initial values,

wherein calculation processes including two-electron integrations on the density submatrixes are executed in parallel at [[each]] the plurality of the nodes while the multiple density submatrixes are being sequentially transferred between the multiple nodes via said communication device, wherein, in each of the computers, the density submatrixes stored in the matrix storage is transferred to one of other computes according to order of transfer, and the density submatrixes which are transferred thereto are store in the matrix storage,

wherein the execution of the calculation processes and transferring are repeated at the number of times which corresponds to the number of the nodes to subject all of the density submatrixes to the calculation processes, and

wherein a resultant Fock matrix of the target molecule is can be obtained by adding an H-core matrix to the combination of combining resultant [[Fock]] submatrices stored in said matrix storages of said plurality of nodes.

14. (Canceled).

15. (Currently Amended) The method according to Claim 1, further comprising: computing, using the ~~multiple density submatrixes being transferred between said plurality of computers~~ the obtained Fock matrix of the target molecule, precise simulations of structures and physical properties of ~~molecules~~ the target molecule, and chemical bonds, molecular orbitals and electron states in ~~molecules~~ the target molecule, wherein no high-performance computers are included in said plurality of computers making up the computer cluster.

16. (Canceled).

17. (Currently Amended) The system according to Claim 7, wherein the ~~multiple density submatrixes are transferred between said plurality of computers, so as~~ obtained Fock matrix of the target molecule is used to obtain precise simulations of structures and physical properties of ~~molecules~~ the target molecule, and chemical bonds, molecular orbitals and electron states in ~~molecules~~ the target molecule, and wherein no high-performance computers are included in said plurality of computers making up the computer cluster.

18. (Currently Amended) The computer readable storage medium according to Claim 13, wherein the ~~multiple density submatrixes are transferred between said plurality of computers, so as~~ obtained Fock matrix of the target matrix is used to obtain precise simulations of structures and physical properties of ~~molecules~~ the target molecule, and chemical bonds, molecular orbitals and electron states in ~~molecules~~ the target molecule, and wherein no high-performance computers are included in said plurality of computers making up the computer cluster.

19. (Canceled).